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Trying to constrain the location of the QCD critical endpoint with lattice simulations

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Abstract

We discuss the reliability of available methods to constrain the location of the QCD critical endpoint with lattice simulations. In particular we calculate the baryon fluctuations up to χ_8^B using simulations at imaginary chemical potentials. We argue that they contain no hint of criticality.

Keywords: lattice QCD, phase diagram, finite density

1. Introduction: Lee-Yang zeros and a toy study at $N_t = 4$

The equation of state of QCD matter at $\mu = 0$ has been calculated with lattice QCD techniques [1, 2, 3]. Calculating the equation of state also for nonzero density is a difficult task, because of the sign and overlap problems. The state-of-the-art at the moment for realistic lattices is to calculate Taylor coefficients of the pressure [4, 5, 6, 7, 8] either by direct calculations at $\mu = 0$ or via fitting a Taylor ansatz to lattice simulation results at zero and imaginary chemical potentials. There exist now lattice calculations of higher order fluctuations χ_6^B and χ_8^B for fine lattices, though the statistical error bars on χ_8^B are still quite large. It is a natural and important question to ask, whether these recent lattice results show any remnants of criticality. In this conference contribution we will examine this question in some detail.

The grand canonical partition function at finite volume in the latticce is a finite order polynomial in $e^{\mu_q/T}$:

$$\mathcal{Z}(\mu_q^2, T) = \sum_{N=-N_s^3}^{+N_s^3} Z_N(T) e^{N3\mu_q/T} \tag{1}$$

[1] speaker

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Since it is a polynomial, it is guaranteed to have roots, called the Lee-Yang zeros. It is also an even function in μ_q, making the natural variable μ_q^2. The infinite volume limit of the Lee-Yang zeros gives important information about the thermodynamics of a system. Here we concentrate on the Lee-Yang zero closest to zero, and call it μ_{LY}^2. If we have a nonzero infinite volume limit of $\mathrm{Im}\,\mu_{\mathrm{LY}}^2$ we have an analytic crossover. In this case $\mathrm{Im}\,\mu_{\mathrm{LY}}^2$ can be thought of as a measure of the strength of the crossover. For a genuine phase transition, we expect the infinite volume limit of the Lee-Yang zero to be real. For any finite volume, the convergence radius of the Taylor expansion of the pressure in μ_q^2 is given by the distance of the closest Lee-Yang zero to $\mu_q = 0$.

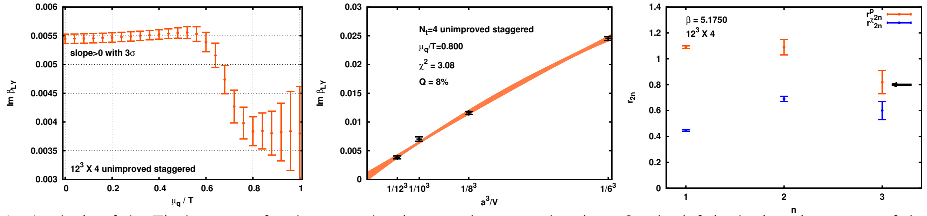

Fig. 1. Analysis of the Fischer zeros for the $N_t = 4$ unimproved staggered action. On the left is the imaginary part of the closest Fischer zero as a function of the quark chemical potential for the $12^3 \times 4$ lattice. On the center is the infinite volume extrapolation for $\mu_q/T = 0.2$. On the right are the ratio estimators for the pressure $r_{2n}^p = \left|\frac{(2n+2)(2n+1)\chi_{2n}^B}{\chi_{2n+2}^B}\right|^{1/2}$ and the baryon number susceptibility $r_{2n}^\chi = \left|\frac{2n(2n-1)\chi_{2n}^B}{\chi_{2n+2}^B}\right|^{1/2}$ on a $12^3 \times 4$ lattice. One can see that the ratio estimators are in the same ballpark as the critical endpoint estimate from the analysis of the Fischer zeros, indicated by an arrow on the right.

For coarse lattices, there exists algorithms to search for the Lee-Yang zeros, or the analogous zeros in gauge coupling parameter β, called the Fischer-zeros β_{LY}. In 2004, such a study led to an estimate of the QCD critical end point on a coarse $N_t = 4$ unimproved staggered lattice [9, 10]. We have repeated the old study, but with a factor of 50 higher statistics and an exact algorithm and found a result very much consistent with the old one. The result on the Fischer zeros on a $12^3 \times 4$ lattice, the infinite volume extrapolation at $\mu_q/T = 0.2$ and the comparison with the ratio estimators for the convergence radius can be seen in Fig. 1. Here the convergence radius estimates from the ratio estimators are in the same ballpark as the critical point estimate from the analysis of β_{LY}.

The algorithms calculating the Fischer or Lee-Yang zeros are prohibitively expensive for more realistic lattices, there the only information available is the first few coefficients of the Taylor series.

2. Ratio estimators for fine staggered lattices

We know present our results for the ratio estimators for a fine $N_t = 12$ 4stout-improved staggered lattice. The 4stout action was introduced in [13]. The details of the lattice calculation of the baryon fluctuations are explained in [8]. Here, we only give a brief description of some features relevant for our discussion. The calculation uses simulations at imaginary chemical potentials [11, 12], where the value of the fluctuations $\chi_1^B, \chi_2^B, \chi_3^B$ and χ_4^B is calculated. We then fit to these values with a Taylor ansatz of the pressure truncated at tenth order:

$$p(T, \mu_B) = p_0(T) + \frac{1}{2!}\chi_2^B(T)\cdot\mu_B^2 + \frac{1}{4!}\chi_4^B(T)\cdot\mu_B^4 + \cdots + \frac{1}{10!}\chi_{10}^B(T)\cdot\mu_B^{10} \quad (2)$$

The fit is performed with a Bayesian procedure, where the higher order fluctuations χ_8^B and χ_{10}^B have a prior. This prior allows for the HRG prediction but does not prefer it, it also allows for the coefficients to grow faster than in the HRG, which could be interpreted as a signal for critical behavior. More precisely, in the HRG we have $\chi_{2n+2}^B/\chi_{2n}^B = 1$ and therefore the ratio estimator for the susceptibility χ_2^B grow as $r_{2n}^\chi \equiv \left|\frac{2n(2n-1)\chi_{2n}^B}{\chi_{2n+2}^B}\right|^{1/2} = \sqrt{2n(2n-1)}$. To have a finite radius of convergence on therefore needs the coefficients to grow like $\frac{\chi_{2n+2}^B}{\chi_{2n}^B} \sim n^2$. We instead see for the first few coefficients a result consistent with HRG.

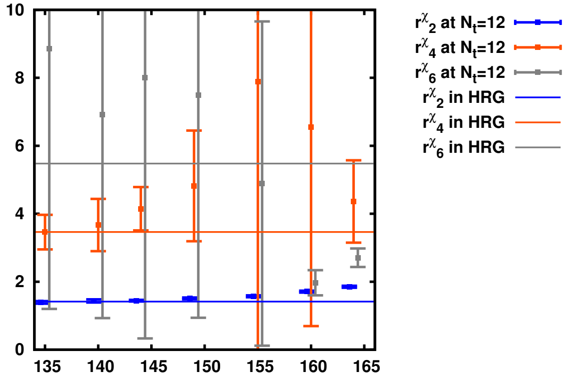

Fig. 2. Ratio estimators of the susceptibility $r^{\chi}_{2n} \equiv \left|\frac{2n(2n-1)\chi^B_{2n}}{\chi^B_{2n+2}}\right|$ on an $N_t = 12$ 4stout-improved staggered lattice.

3. A closer look at the lattice results for $N_t = 12$

To shed some light on the previous result consider the following toy model. Start with some parametrization of the curve χ^B_1/μ_B as a function of T at $\mu = 0$. Assume that the only difference in the physics at finite μ is a shift in this curve in the T direction. The inflection point of this curve is one possible definition of T_c, so shift this curve by using the curvature κ of the cross-over line found in the literature. This gives a model prediction of χ^B_1 for any finite μ, and by differentiation at zero chemical potential, it also gives predictions of χ^B_4, χ^B_6 and χ^B_8. Comparison of this toy model with the actual lattice data is shown in Fig. 2.

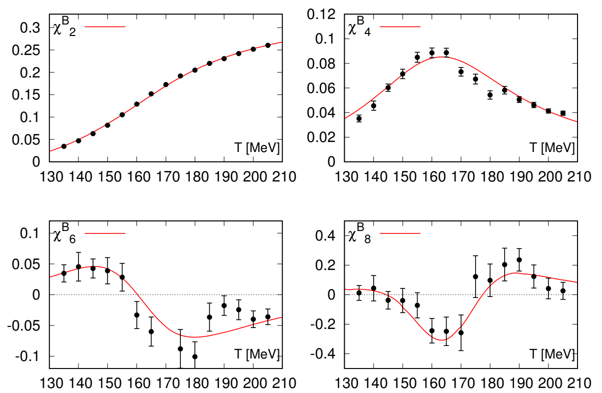

Fig. 3. Comparison of the simple toy model described in the text, with the actual lattices simulations.

The discussion of this toy model suggests the following non-trivial consequence for modeling: In order to reproduce the lattice data on $\chi^B_2, \chi^B_4, \chi^B_6$ and χ^B_8 at the present accuracy all a model has to do is to reproduce χ^B_2 and the curvature of the cross-over line κ, without the crossover getting stronger already at low values of the chemical potential. As long as these conditions are met, the features of the higher order baryon number susceptibilities will be automatically reproduced.

Among other things, this discussion suggests that near and above T_c, the curvature of the crossover implies $r^{\chi}_2 < r^{\chi}_4$ and $r^{\chi}_4 > r^{\chi}_6$, a feature clearly visibly on the lattice data at $T = 165$MeV. Here the closest Lee Yang zero most likely has a large imaginary part, and the ratio estimator is not expected to give a good estimate of the radius of convergence.

As the existence of κ implies $r^{\chi}_4 > r^{\chi}_6$ near or slightly above T_c, while the HRG $r^{\chi}_4 < r^{\chi}_6$, by continuity, there must be a temperature $T_* < T_c$ where $r^{\chi}_4 = r^{\chi}_6$. This is an apparent convergence in the first few ratio estimators, that however does not imply anything about criticality, and when the statistical errors get small enough to see T_* one should be careful not to misinterpret this apparent convergence.

An other explicit example of a model reproducing the lattice data on baryon fluctuations, but having no critical point is found in [14, 15]. Obviously, this does not necessarily mean that there is no critical point, just that if it exists than at the current levels of statistical uncertainty, the lattice results are not sensitive to it.

In summary, if a critical point is close to zero chemical potential, one may see it in a fast convergence of radius of convergence estimators, this might be what is happening for $N_t = 4$. On the other hand, apparent convergence does not imply a critical point. In fact, we argued that even in the case with no CEP, the ratios r_4^χ and r_6^χ will show apparent convergence somewhere below T_c. For our fine lattice ($N_t = 12$ 4stout) the sign structure of χ_6^B and χ_8^B near T_c is consistent with only a κ and no criticality. At lower temperatures the data quickly become compatible with the HRG model, showing no traces of criticality. Finally we note that none of these observations can be converted into a rigorous bound for the convergence radius of the Taylor series.

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